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NUMERICAL SIMULATION OF AN IN-SITU COMBUSTION MODEL FORMULATED AS MIXED COMPLEMENTARITY PROBLEM

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Abstract. *The difficulty of the extraction of medium and heavy oil is its hight viscosity. One form of decreasing it consists in applying the thermal methods as steam injection or in-situ combustion. In the present work one simple model for in-situ combustion is presented. It consists of two nonlinear partial differential equations. As obtaining the analytical solutions for this type of equation is near impossible, it is necessary to make computational simulations. In fact, the solutions for in-situ combustion problem involves shock waves, which increases the difficulty of the numerical simulations. A possible way to avoid this problem is to rewrite the differential equations as one mixed nonlinear complementarity problem. In this work numerical simulations are performed using the finite difference method and a feasible directions algorithm for mixed nonlinear complementarity problem to obtain approximate solutions of the proposed model. The results are compared with ones obtained by using the Newton's method that was used in other references.*

Keywords: *In situ combustion, Conservation laws, Mixed complementarity problem.*

1 INTRODUCTION

Parabolic problems that can be written as a variational problem involving a complementarity condition and moving boundaries appear in several applications, as described in Chapiro et al. (2016) and references therein. In Chapiro et al. (2016) was presented a general technique for moving boundary problems, that can be written as a nonlinear complementarity problem (NCP). For $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$ a nonlinear vector function, we search for $u \in D \subset \mathbb{R}^n$ such that:

$$F(u) \geq 0, \;\; u \geq 0 \quad \text{and} \quad u \circ F(u) = 0, \tag{1}$$

where " $\circ$ " represents the Hadamard product and $u \geq 0$ means that each component of the vector u is nonnegative. In the present text this technique is extended to the mixed nonlinear complementarity problem (MNCP). For $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ and $Q : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ continuously differentiable vector functions, we search $(x, y) \in \mathbb{R}^n \times \mathbb{R}^m$ such that:

$$F(x, y) \geq 0, \;\; x \geq 0, \;\; x \circ F(x, y) = 0 \quad \text{and} \quad Q(x, y) = 0. \tag{2}$$

These numerical methods are based on a combination of the Crank-Nicolson finite difference scheme, Strikwerda (1989), and a globally convergent Mazorche and Herskovits (2005). As a result the moving boundary is obtained naturally, without need of regularizations unlike from other methods. The robustness of the algorithm allows longer time steps implying in better convergence as shown in our preliminary results, see Chapiro et al. (2010). Other methods dealing with complementarity problems can be found in Chen and Mangasarian (1996), Gharbia and Jaffré (2014), Lauser et al. (2011), Mazorche and Herskovits (2005). The present techniques are appropriate for practical applications since it brings together classical numerical techniques for PDEs with a robust and efficient interior point algorithm having a complete a theoretical fundamentation and good numerical results.

This paper is organized as follows. In Section 2 we describe the nonlinear complementarity algorithm and mixed nonlinear complementarity algorithm employed at each time step and the finite difference scheme used for time evolution. In Section 3 we introduce the model describing in-situ combustion and study rigorously the non-combustion waves. In Section 4 we present numerical results for in-situ combustion using finite difference esqueme (FDS). Finally, in Section 5 we present some conclusions and discussions.

2 THE NUMERICAL METHOD

In this section we describe our approach to solve the system of parabolic partial differential equations numerically. We use FDS for space discretization and a Feasible Direction Algorithm applied to Nonlinear Complementarity Problem (FDA–NCP) as presented in Chapiro et al. (2016) and the same algorithm applied to the Mixed Nonlinear Complementarity Problem (FDA–MNCP) as its natural extension. Both algorithms solve the discrete problem at each time step and its implementation is flexible, since we can change the space discretization and the algorithm independently. Next we present a brief description of both algorithms.

2.1 The Nonlinear Complementarity Algorithm

As presented in Chapiro et al. (2016), FDA–NCP is an iterative algorithm used to solve Eq. (1). It starts from an initial point in int(Υ) and generates a sequence of points also in int(Υ) that converges to the required solution, where $\Upsilon = \{u \in \mathbb{R}^n \ : \ u \geq 0, F(u) \geq 0\}$ is the feasible set and int(Υ) its interior. Then, at each point it defines a feasible direction that is also a descent direction for the potential function $\Phi(u) = \sum_{i=1}^{n} u_i \, F_i(u)$. On that direction a new interior point with a lower potential is obtained. That point is defined to be the next point of the sequence and the algorithm returns to the first step till a convergence criterion is satisfied. The search direction is based on Newton's direction for the nonlinear system of equations $u \circ F(u) = 0$. To obtain feasibility, Newton's direction is modified by a restoration direction, as done in Herskovits (1998).

The following notation will be employed to describe the algorithm FDA–NCP: $F^k = F(u^k)$, $M^k = \nabla(u^k \circ F(u^k))$, $\Phi^k = \Phi(u^k)$, $\nabla\Phi^k = \nabla\Phi(u^k)$ and $\mu^k = \Phi^k/n$.

FDA–NCP Algorithm
Data: $u^0 \in \text{int}(\Upsilon)$, $k = 0$, $\epsilon > 0$, $E = [1, ..., 1]^T$, $\nu, \nu_1 \in (0, 1)$, $\alpha \in (0, 1/2)$.
Step NCP-1: Compute the search direction d^k by solving $M^k \, d^k = -u^k \circ F^k + \alpha \, \mu^k \, E$.
Step NCP-2: Armijo line search. Set t^k as the first number in the sequence $1, \nu, \nu^2, \nu^3, ...$ that satisfies:
$u^k + t^k \, d^k \geq 0$, $F(u^k + t^k \, d^k) \geq 0$ and $\Phi(u^k + t^k \, d^k) \geq \Phi^k + t^k \, \nu_1 \, (\nabla\Phi^k . d^k)$.
Step NCP-3: Update. Set $u^{k+1} = u^k + t^k \, d^k$ and $k = k + 1$.
Step NCP-4: Stopping criterion: if $\|u^k \circ F^k\| \leq \epsilon$ stop, else go to step 1.

2.2 The mixed nonlinear complementarity algorithm

FDA–MNCP is an iterative algorithm used for solving Eq. (2). Analogously to FDA–NCP, it starts from an initial point in int(Υ) and generates a sequence of points also in int(Υ), where: $\Upsilon = \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^m | x \geq 0 \, , F(x, y) \geq 0\}$. This algorithm defines a feasible direction that is also a descent direction for the potential function $f(x, y) = \Phi(x, y) + ||Q(x, y)||^2$ where $\Phi(x, y) = \sum_{i=1}^{n} x_i \, F_i(x, y)$. The search direction is based on Newton's direction for the nonlinear system of equations $S(x, y) = 0$ where $S(x, y) = (x \circ F(x, y), \ Q(x, y))^T$.

FDA-MNCP Algorithm
Parameters:
$c > 0$, $\alpha, \eta, \nu \in (0, 1)$, $\beta \in (1, 2]$ and $\rho_0 < \alpha \min\{1, 1/(c^{\beta-1})\}$.
$\epsilon > 0$, $E_0 = [0, ..., 0]^T \in \mathbb{R}^m$, $E_1 = [1, ..., 1]^T \in \mathbb{R}^n$.
Initial Data: $(x^0, y^0) \in \text{int}(\Upsilon)$ such that $f(x^0, y^0) < c$ and $k = 0$.

Step MNCP-1: Compute the search direction $d^k = \begin{pmatrix} d_x^k \\ d_y^k \end{pmatrix}$ by solving

$$\nabla S(x^k, y^k) d^k = \begin{pmatrix} -x^k \circ F(x^k, y^k) + \rho^k E_1 \\ -Q(x^k, y^k) \end{pmatrix} , \tag{3}$$

where $\rho^k = \rho_0 \frac{\phi^\beta(x^k, y^k)}{n}$.

Step MNCP-2: Armijo line search. Set t^k as the first number in the sequence $1, \nu, \nu^2, \nu^3, ...$ that satisfies

$$x^k + t^k d_x^k \geq 0; \tag{4}$$

$$F(x^k + t^k d_x^k, y^k + t^k d_y^k) \geq 0; \tag{5}$$

$$f(x^k + t^k d_x^k, y^k + t^k d_y^k) \leq f(x^k, y^k) + t^k \eta \nabla f(x^k, y^k)^t d^k; \tag{6}$$

Step MNCP-3: Update. Set $(x^{k+1}, y^{k+1}) := (x^k + t^k d_x^k, y^k + t^k d_y^k)$ and $k := k + 1$.
Step MNCP-4: Stopping criterion: if $\|f(x^k, y^k)\| \leq \epsilon$ stop, else go to step 1.

The present algorithm is very simple to implement and requires a computer effort similar to that of Newton method for nonlinear systems of equations.

For both algorithms the strong theoretical results are presented in Herskovits and Mazorche (2009), Mazorche and Herskovits (2005) proving that the search direction d^k is well defined in Υ, the global convergence is guaranteed and if $t^k = 1$ for large k the algorithm rate of convergence is quadratic.

3 IN-SITU COMBUSTION

In this section we address a simple in-situ combustion model described by a system of two nonlinear differential equations, see Chapiro et al. (2016). It is a simplified model derived from Akkutlu and Yortsos (2003), Chapiro et al. (2012). In dimensionless form the model is written as

$$\frac{\partial \theta}{\partial t} + u\frac{\partial(\rho\theta)}{\partial x} = \frac{1}{\mathrm{Pe}_T}\frac{\partial^2 \theta}{\partial x^2} + \Phi, \tag{7}$$

$$\frac{\partial \eta}{\partial t} = \Phi, \tag{8}$$

$$\rho = \theta_0/(\theta + \theta_0), \tag{9}$$

$$\Phi = \beta(1-\eta)\exp\left(-\frac{\mathcal{E}}{\theta + \theta_0}\right), \tag{10}$$

where θ is the scaled temperature, η represents immobile fuel depth as commonly used in oil engineering ($\eta = 1$ means no fuel and $\eta = 0$ means maximum fuel). Here Pe_T is the Peclet number for thermal diffusion, u is the dimensionless gas speed, $\mathcal{E}$ is the scaled activation energy and θ_0 is the scaled reservoir temperature. Typical values of the quantities in Eq. (7)-Eq. (10) are given in Section 4. The system must be solved with the initial reservoir conditions

$$t = 0,\ x \geq 0: \quad \theta = 0,\ \ \eta = 0, \tag{11}$$

and the left boundary conditions corresponding to the injection conditions

$$t \geq 0,\ x = 0: \quad \theta = 0,\ \ \eta = 1. \tag{12}$$

The dimensionless parameter values are $\mathrm{Pe}_T = 1406$, $\beta = 7.44 \cdot 10^{10}$, $\mathcal{E} = 93.8$, $\theta_0 = 3.67$ and $u = 3.76$.

In order to represent the System Eq. (7)-Eq. (8) in a mixed complementarity form we make a transformation similar to Chapiro et al. (2016) (see also Gharbia and Jaffré (2014)), obtaining

$$\theta \geq 0,\ \eta \in \mathbb{R}: \quad \frac{\partial \theta}{\partial t} + u\frac{\partial(\rho\,\theta)}{\partial x} - \frac{1}{Pe_T}\frac{\partial^2 \theta}{\partial x^2} - \Phi \geq 0, \tag{13a}$$

$$\frac{\partial \eta}{\partial t} - \Phi = 0, \tag{13b}$$

$$\left(\frac{\partial \theta}{\partial t} + u\frac{\partial(\rho\,\theta)}{\partial x} - \frac{1}{Pe_T}\frac{\partial^2 \theta}{\partial x^2} - \Phi\right)\theta = 0, \tag{14a}$$

We need Eq. (14) to be satisfied at the right end of the interval, where Eq. (7) may not be satisfied. This explains the choice of dimensionless variable η describing fuel depth inside the reservoir.

3.1 Non-Combustion Waves

Apart of the combustion wave, the solution of System (7)-(9) possesses non-combustion waves, which can be studied analytically and used to validate numerical simulations. We consider a hyperbolic part of System (7)-(9) obtained by neglecting the reaction terms and second derivatives, see Chapiro et al. (2012) and references therein.

$$\frac{\partial \theta}{\partial t} + u\frac{\partial}{\partial x}\left(\frac{\theta_0 \theta}{\theta + \theta_0}\right) = 0, \qquad \frac{\partial \eta}{\partial t} = 0. \tag{15}$$

The equations above form a system of conservation laws and can be solved for the corresponding Riemann problem, i.e., considering the initial data given by the discontinuous step function. Typically, the solution of a Riemann problem is a train of waves, which can be shocks, rarefaction or contact discontinuities. This solution is physically admissible if it satisfies the entropy conditions, see LeVeque (1992) for details.

Theorem 1 *The solution of System* (15) *with initial data given by*

$$(\theta(x,0), \eta(x,0)) = \begin{cases} (\theta_l, \eta_l), & x \leq 0 \\ (\theta_r, \eta_r), & x > 0 \end{cases} \tag{16}$$

where θ_l, η_l, θ_r and η_r are constants satisfying $\theta_l \leqslant \theta_r$ can contain:
(1) a Lax entropic contact wave satisfying $\theta_l = \theta_r$ and $\eta_r \geq 0$ with velocity equal to zero;
(2) a Lax entropic shock wave satisfying $\eta_l = \eta_r$ and $\theta_r \geq 0$ with velocity

$$s = \frac{u\theta_0^2}{(\theta_r + \theta_0)(\theta_l + \theta_0)}. \tag{17}$$

This theorem was proved in Chapiro et al. (2016).

4 NUMERICAL SOLUTION OF IN-SITU COMBUSTION MODEL

In this section we present numerical results using FDS + FDA–MNCP algorithm and validate the solution obtained with FDS + Newton's method.

We consider an homogeneous grid for the variable x with $M+1$ points, where x_0 and x_M are the boundary points of the interval of the calculation. The grid spacing is $h = x_{m+1} - x_m = 1/M$ and the grid position m corresponds to $x = m\Delta x$. Analogously the time is denoted by t with the time index denoted by n and the time step is Δt.

In order to solve our problem we employ the following scheme
Step 0: We start with the initial variable u_m^0, $m = 0, 1, \ldots, M$ and the first time step Δt_0.
Step 1: Obtain the discrete form of Eq. (2) using FDS.
Step 2: Use FDA–MNCP algorithm to solve the mixed nonlinear complementarity problem from step # 1.
Step 3: Use the solution from **step 2** as the variable u value at the next time step. Repeat the algorithm from the **step 1** until reaching the final time.

The global properties do the Crank-Nicolson scheme are well known, e.g. Morton and Mayers (2005). In general, the convergence of FDS is rigorously proved only for simple equations or linear systems, see Strikwerda (1989), however they are widely used for solving numerically reaction-diffusion equations similar to the examples addressed here, see Bruining et al. (2009), Chapiro et al. (2012, 2010), Gupta and Kumar (1981), Gupta (2015).

4.1 Numerical simulation of in-situ combustion using FDS

Let be $F(\theta, \eta)$ and $Q(\theta, \eta)$ the differential operators corresponding to the left side of inequality (13). We write them in the discrete form, using Crank-Nicolson scheme

$$\begin{aligned} F_\Delta(\theta,\eta) = \theta_m^{n+1} - \theta_m^n + u\Delta t \frac{\rho_{m+1}^{n+1}\theta_{m+1}^{n+1} - \rho_{m-1}^{n+1}\theta_{m-1}^{n+1}}{4\Delta x} + u\Delta t \frac{\rho_{m+1}^{n}\theta_{m+1}^{n} - \rho_{m-1}^{n}\theta_{m-1}^{n}}{4\Delta x} \\ - \frac{\Delta t}{\mathrm{Pe}} \frac{\theta_{m-1}^{n+1} - \theta_m^{n+1} + \theta_{m+1}^{n+1}}{2\Delta x^2} - \frac{\Delta t}{\mathrm{Pe}} \frac{\theta_{m-1}^{n} - 2\theta_m^{n} + \theta_{m+1}^{n}}{2\Delta x^2} - \frac{\Delta t(\Phi_m^{n+1} + \Phi_m^n)}{2}, \end{aligned} \tag{18}$$

$$Q_\Delta(\theta,\eta) = \eta_m^{n+1} - \eta_m^n + \frac{\Delta t(\Phi_m^{n+1} + \Phi_m^n)}{2}. \tag{19}$$

Same discretization was employed in Chapiro et al. (2012, 2014) to simulate more general and complex combustion models. The results showed good agreement when compared with analytical solutions.

Substituting the differential operator $F(\theta, \eta)$ and $Q(\theta, \eta)$ in (13) by the discrete operators $F_\Delta(\theta, \eta), Q_\Delta(\theta, \eta)$ and isolating the terms for time step $n+1$ on the left, we obtain the system of equations describing time evolution. The evaluation equation for the grid points $m = 0$ and $m = M$ can be described using the boundary conditions.

The boundary conditions impose constant temperature and no fuel at the left end of the interval, $x_0 = 0$. That is $\theta(x_0, t) = 0$ and $\eta(x_0, t) = 1$, $t \geq 0$. As there is no fixed right point, the boundary conditions at the right are modeled as zero flow Neumann boundary conditions.

To compare the FDS + Nonlinear Complementarity algorithm with the classical FDS + Newton's method, four different simulations were performed inside the interval $[0, 0.05]$ using constant time step k and space grids with 51 ($k = 10^{-5}$), 101 ($k = 5 \cdot 10^{-6}$), 201 ($k = 2.5 \cdot 10^{-6}$) and 401 ($k = 1.25 \cdot 10^{-6}$) points, see Figures 1 (a), (b), (c) and (d).

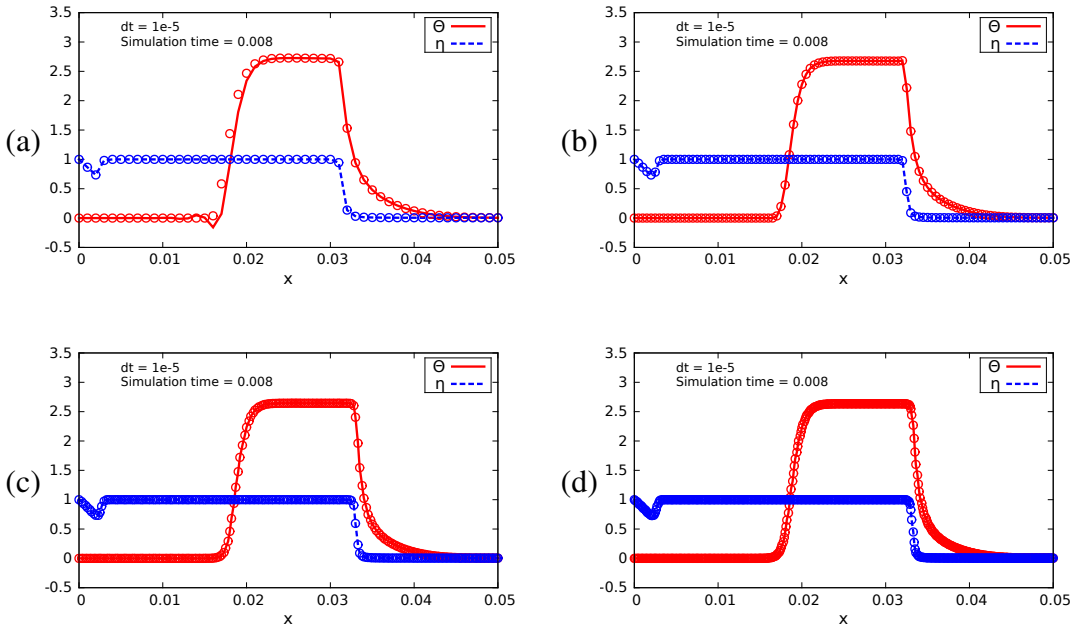

Figure 1: The solution obtained with FDS + Newton (lines) is compared to one obtained with FDS + FDA–MNCP (circles). Solutions at time $t = 0.008$ are shown in (a), (b), (c) and (d) corresponding to grids with 51, 101, 201 and 401 points.

As one can see in Fig. 1, the proposed algorithm shows better results than the finite difference scheme with Newton's method. In Fig. 1 (a) the simulation with Newton's method and 51 points grid shows dispersion effect. This effect increases when more sparse grid is used turning Newton's method divergent. On the other hand, the technique using FDA–MNCP converges even with 25 points grid.

When we compare FDS + FDA–NCP and FDS + Newton'method in Fig. 2, we can observe the same effect as in Fig. 1. In Chapiro et al. (2016) was presented the comparison between the simulations using FEM + FDA–NCP and FEM + Newton's method and also the relative error analysis was made.

In Fig. 3, we compare the numerical results obtained by using FDS + FDA–MNCP with the results obtained by using FDS + FDA–NCP. We can see that the solutions are almost identical. Notice that the solutions are always positive.

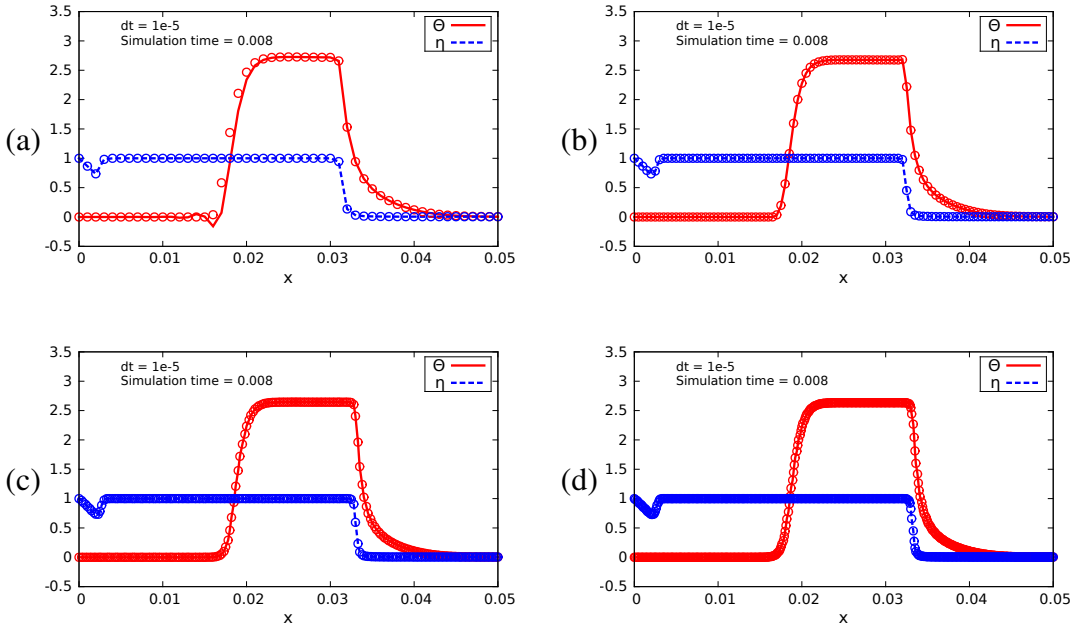

Figure 2: The solution obtained with FDS + Newton (lines) is compared to one obtained with FDS + FDA–NCP (circles). Solutions at time $t = 0.008$ are shown in (a), (b), (c) and (d) corresponding to grids with 51, 101, 201 and 401 points.

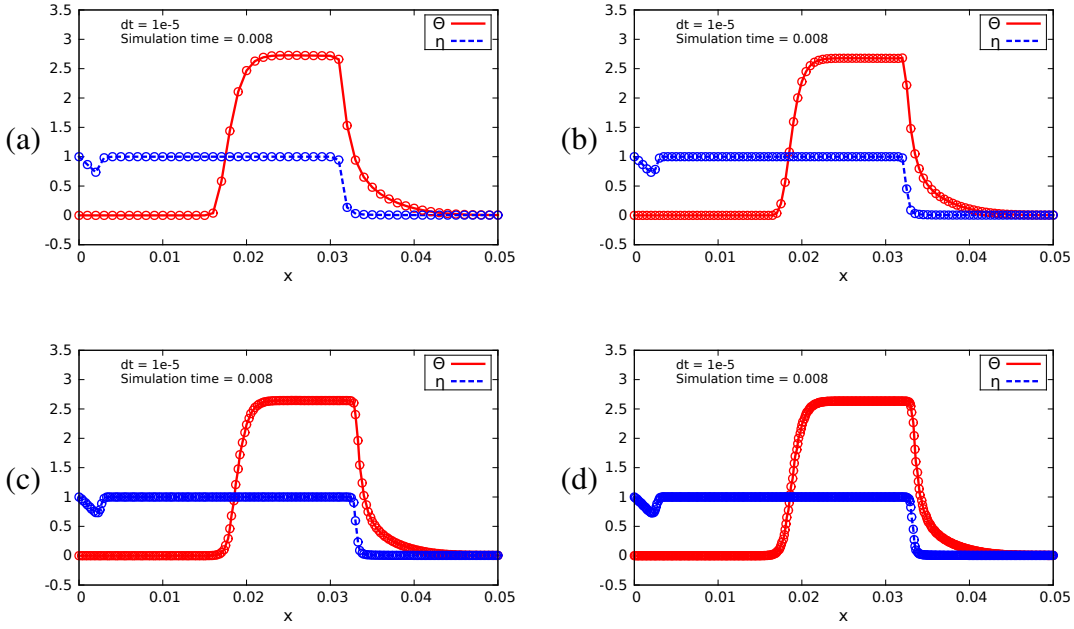

Figure 3: The solution obtained with FDS + FDA–NCP (lines) is compared to one obtained with FDS + FDA–MNCP (circles). Solutions at time $t = 0.008$ are shown in (a), (b), (c) and (d) corresponding to grids with 51, 101, 201 and 401 points.

5 CONCLUSIONS

In all the iterations the FDA–MNCP algorithm had a line search step approximating to 1 near the solution as expected from the theoretical results presented in Section 2.2. This fact indicates that the FDA-MNCP algorithm converges quadratically.

The feasible directions algorithm (FDA-MNCP) is a simple, efficient and robust algorithm for mixed nonlinear complementarity problems and converged for all time steps in all test problems. This algorithm needs less grid points than FDA-NCP and it also converges in less time because it involves smaller linear systems.

The main advantage in using the FDA–MNCP is the fact that the moving boundary is obtained directly as a solution of the mixed complementarity problem. This approach has a potential advantage over the Newton's method where the moving boundary is difficult to obtain due to discontinuities of the solution.

In-situ combustion was modeled using mixed complementarity formulation with moving boundary, which can be an interesting approach for general flow in porous medium. Our numerical results show good agreement with direct numerical simulations using Newton's method and FDA–MNCP combined with FDS as shown in Fig. 1 and, FDA–NCP and FDA–MNCP combined with FDS is shown in Fig. 3. The non-combustion waves that were obtained numerically are very similar to those given by the analytical study presented in Section 3.1.

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